Asymptotic Freedom and Bound States
in Hamiltonian Dynamics

June 1997

Stanisław D. Głazek

Institute of Theoretical Physics, Warsaw University
ul. Hoża 69, 00-681 Warsaw

Kenneth G. Wilson

Department of Physics, The Ohio State University
Columbus, Ohio 43210-1106

Abstract

We study a model of asymptotically free theories with bound states using the similarity renormalization group for hamiltonians. We find that the renormalized effective hamiltonians can be approximated in a large range of widths by introducing similarity factors and the running coupling constant. This approximation loses accuracy for the small widths on the order of the bound state energy and it is improved by using the expansion in powers of the running coupling constant. The coupling constant for small widths is order 1. The small width effective hamiltonian is projected on a small subset of the effective basis states. The resulting small matrix is diagonalized and the exact bound state energy is obtained with accuracy of the order of 10% using the first three terms in the expansion. We briefly describe options for improving the accuracy.

PACS Numbers: 11.10.Gh

1. INTRODUCTION

So far, we do not have a precise theoretical description of the bound states of quarks and gluons in QCD which could simultaneously explain the parton model and the constituent quark model of hadronic structure. In particular, QCD is asymptotically free and the perturbative running coupling grows at small momentum transfers beyond limits. This rise invalidates the usual perturbative expansion in the region of scales where the bound states are formed.

Ref.[1] suggested a light-front hamiltonian approach to this problem which is based on the calculation of the effective hamiltonians using the similarity renormalization group. [2] [3] Besides the calculation of the hadronic spectrum, one of our purposes is to obtain the quark bound state wave functions that can be used in the parton models of large momentum transfer processes. An alternative approach is the lattice gauge theory which is making progress but does not easily yield such wave functions. [4] Other recent research in the renormalized light-front hamiltonian approach to QCD is described in Ref. [5].

Wegner [6] proposed a flow equation for hamiltonians in solid state physics which is of the same kind as in the similarity renormalization group. Wegner's equation is based on an explicit form for the generator of the similarity transformation and corresponds to the Gaussian similarity factor with a uniform width.

This paper describes a numerical study of the key elements of the hamiltonian approach in a simple matrix model which is asymptotically free, contains a bound state and can be diagonalized exactly. We check the accuracy of different approximations in perturbation theory by comparison with the exact solution. The exact solution for the renormalization group flow of the effective hamiltonians in the matrix model is obtained numerically using Wegner's equation.

We start from the general assumption that the asymptotically free theories have many degrees of freedom which are characterized by different scales of energy as measured by certain H_0. Then, we define matrix elements of the initial interaction hamiltonian H_I between eigenstates of H_0.

The model we study can be alternatively derived by discretization of the 2-dimensional Schrödinger equation with a potential of the form a coupling constant times a δ-function.[7] The continuous version of the 2-dimensional model has been studied by many authors. The discretized version was analyzed in Ref. [8] using the exact solution to Wegner's equation. It was shown there that the Wegner equation has the renormalization group interpretation.

This paper is organized as follows. In Section 2 we describe the model. The parameters are chosen in a way which will make it clear that the method of solution we use may have a wide range of other applications. Numerical results for the effective hamiltonians are presented in Section 3. We discuss the approximation based on the similarity factors and the running coupling constant and we describe results obtained in perturbation theory. Section 4 concludes the paper with a discussion of some options for improvements in perturbative calculations of the effective hamiltonians in the range of widths near the bound state formation scale.

2. MODEL

The hamiltonian H_0 is assumed to have a finite discrete set of eigenstates,

$$H_0|i> = E_i|i> . \tag{2.1}$$

The eigenstates are orthogonal and normalized,

$$<i|j> = \delta^{ij} . \tag{2.2}$$

The dynamics of states in the space spanned by this set is defined by the interaction hamiltonian, H_I, whose matrix elements are assumed to be

$$<i|H_I|j> = -g\sqrt{E_iE_j} , \tag{2.3}$$

where g is a dimensionless coupling constant. The whole hamiltonian is denoted by H, $H = H_0 + H_I$.

In the current study, we choose the eigenvalues of H_0 in the form

$$E_i = b^{2i} . \tag{2.4}$$

In the numerical calculations we use $b = \sqrt{2}$. The integer power i ranges from M to N. The integer M is considered to be large and negative. The lower, infrared bound on the free energies is 2^{-M}. The integer N is considered to be large and positive. The upper, ultraviolet free energy bound is given by 2^N. In the numerical study, we use $M = -21$ and $N = 16$.

For the purpose of analogy to QCD, we adopt the convention that the energy equal 1 corresponds to 1 GeV, although the units of energy are arbitrary. Thus, the ultraviolet cutoff corresponds to 65 TeV and the infrared cutoff corresponds to 0.5 eV.

With the above choices, the hamiltonian H is a 38×38 matrix. For the coupling constant $g > 1/38$, the matrix has one negative eigenvalue and 37 positive eigenvalues. The coupling constant is adjusted to obtain the negative eigenvalue equal -1.00000000 or, in our convention, -1 GeV. Namely, $g = 0.06060600631$. The many digits are given for readers interested in the numbers.

The eigenstate with the negative eigenvalue corresponds to the s-wave bound state in the continuum Schrödinger equation with the δ-potential. The positive eigenvalue eigenstates correspond to the s-wave scattering states. We refer the reader to the work of Jackiw [7] for details. The only new steps required are the replacement of the continuous energy scale in Ref. [7] by the discrete one in Eq. (2.4) and the introduction of the infrared and ultraviolet cutoffs. These steps are described in Ref. [8].

To verify the ultraviolet renormalizability of the model and its infrared convergence, we have studied a set of exact results for different numbers M and N. The same qualitative results as for $M = -21$ and $N = 16$ can be obtained already for $-M = N = 8$. We have checked the renormalizability by varying the ultraviolet limit N from 4 to 16 and we verified the infrared convergence by varying the limit M from -4 to -21. We have studied in detail the case $-M = N = 12$. The eigenvalues in the latter case are almost the same as the corresponding eigenvalues in the case $M = -21$ and $N = 16$ with the accuracy better than 1% for the extreme eigenvalues. The intermediate eigenvalues match with much higher accuracy, correspondingly. For example, eigenvalues order 1 have the same 5 significant digits in both cases.

We calculate effective hamiltonians using the similarity renormalization group equations in the differential form. The effective hamiltonians are parametrized by their width in energy. The width is denoted by λ.

We use Wegner's flow equation [6] which provides a very elegant definition of the similarity transformation with a uniform band width and an explicit expression for the generating matrix. The effective hamiltonian matrices, $\mathcal{H} \equiv \mathcal{H}(s)$, are parametrized by the parameter s. s ranges from 0 to ∞. Wegner's original notation for this parameter was ℓ instead of s. It will be shown that the hamiltonian width is given by $\lambda = 1/\sqrt{s}$.

The effective hamiltonian is divided into two parts,

$$\mathcal{H} \;\;=\;\; \mathcal{D} + \mathcal{H} - \mathcal{D} \;\;\equiv\;\; \mathcal{D} + \mathcal{V}. \tag{2.5}$$

$\mathcal{D}$ is the diagonal part of the effective hamiltonian matrix,

$$\mathcal{D}_{mn} \;\;=\;\; \mathcal{D}_m \delta_{mn}, \tag{2.6}$$

where $\mathcal{D}_m = \mathcal{H}_{mm}$. $\mathcal{V}$ is the effective interaction. It is equal to the off-diagonal part of the matrix $\mathcal{H}$. The Wegner flow equation is [6]

$$\frac{d\mathcal{H}}{ds} \;\;=\;\; [\,[\mathcal{D}, \mathcal{H}],\, \mathcal{H}\,], \tag{2.7}$$

with the initial condition

$$\mathcal{H}(0) \;\;=\;\; H \,. \tag{2.8}$$

Equations (2.7) and (2.8) ensure that $\mathcal{H}(s)$ is a unitary transform of the initial Hamiltonian H. In terms of the matrix elements, we have

$$\frac{d\mathcal{H}_{mn}}{ds} \;\;=\;\; -(\mathcal{D}_m - \mathcal{D}_n)^2\, \mathcal{V}_{mn} \;\;+\;\; \sum_{\ell}(\mathcal{D}_m + \mathcal{D}_n - 2\mathcal{D}_\ell)\, \mathcal{V}_{m\ell}\, \mathcal{V}_{\ell n}\,, \tag{2.9}$$

Equation (2.9) can be approximately solved for a small coupling constant g by keeping only terms order 1 and g. Namely,

$$\mathcal{H}_{mn}(s) \;\;=\;\; E_m\, \delta_{mn} \;\;-\;\; g\sqrt{E_m E_n}\, \exp\left[-s\,(E_m - E_n)^2\right]\,. \tag{2.10}$$

In this approximation, $\mathcal{D}_m = (1 - g)E_m$. It is clear that the parameter s and the width λ of the similarity renormalization scheme are simply related, $s = \lambda^{-2}$. The similarity factor is a Gaussian function.

It is well known that the coupling constant g must depend on the upper energy bound, 2^N, in order to eliminate the logarithmic divergences in higher orders when $N \to \infty$. Ref. [8] demonstrated that the Wegner flow equation has the standard renormalization group interpretation. Lowering the width $\lambda = s^{-1/2}$ in the discrete model is similar to lowering the upper bound on the energies of the interacting states. Therefore, in the higher order analysis, we replace the coupling constant g in Eq. (2.10) by the running coupling $\tilde{g}(s)$ and use the expansion in $\tilde{g}(s)$ to remove the logarithmic divergences. We will gradually change the notation from the mathematical parameter s to the hamiltonian energy width λ in our parametrization of the effective hamiltonians, including the running coupling constant.

4

The small coupling and large width approximation for $\tilde{g}(s)$ can be derived in the following way. E_m and E_n are very small numbers for m and n close to M. Therefore, Eq. (2.9) for m and n close to M, $g \ll 1$ and s close to 0, reduces to

$$\frac{d\tilde{g}}{ds} = -\tilde{g}^2 \frac{d}{ds} \sum_\ell \exp\left[-2 E_\ell^2 s\right] . \tag{2.11}$$

Integration of Eq. (2.11) for our choice of the model parameters gives the approximate running coupling constant

$$\tilde{g}_a(\lambda) = \frac{g}{1 - g\,(17.4 - \log \lambda^2 / \log 4)} . \tag{2.12}$$

λ is taken in units of GeV. The number 0.4 results from Eq. (2.11), because the contributions of terms with ℓ close to $\log \lambda^2 / \log 4$ are smaller than 1.

Eq. (2.12) implies that the family of the effective theories exhibits typical asymptotic freedom behavior: the coupling gets smaller when the effective cutoff λ is large.

The effective hamiltonians can be written now as

$$\mathcal{H}_{mn}(\lambda) = E_m \delta_{mn} - \tilde{g}_a(\lambda) \sqrt{E_m E_n} \, \exp\left[-[E_m - E_n]^2/\lambda^2\right] + corrections . \tag{2.13}$$

Here, $\mathcal{D}_m(\lambda) = [1 - \tilde{g}_a(\lambda)]E_m + corrections$.

Eq. (2.13) demonstrates the utility of Wegner's equation. However, the uniform width of the effective hamiltonian distinguishes this solution from the widening band structure in the similarity scheme from Refs. [2] and [3]. The widening of the band is useful in high order perturbation theory. A whole class of generalized Wegner equations for the hamiltonian matrix elements can be written which allow the high energy widening of the effective hamiltonian width. Namely,

$$\frac{d\mathcal{H}_\lambda}{d\lambda^2} = \frac{-1}{\lambda^4} \, [F\{\mathcal{H}\}, \mathcal{H}_\lambda] . \tag{2.14}$$

In the original Wegner case, $F\{\mathcal{H}\} = [\mathcal{D}, \mathcal{H}]$. We have made calculations in the model using different formulae for the operation F. For example, we used $[F\{\mathcal{H}\}]_{mn} = \theta[|\Delta_{mn}| - x](|\Delta_{mn}| - x)^k \Delta_{mn} \mathcal{H}_{mn}$, where $\Delta_{mn} = (\mathcal{D}_m - \mathcal{D}_n)/(\mathcal{D}_m + \mathcal{D}_n)$ and x is a function of λ such that $1 > x(\lambda) > x_0 > 0$, (see also Ref. [10]). Nevertheless, we limit the present paper discussion to the application of the original Wegner equation, for simplicity and because no clear advantage of the more general equations over the Wegner equation has been visible in the numerical studies we performed so far.

The structure of Eq. (2.10) demonstrates that the approximate solution including the running coupling cannot be obtained in the first order perturbation theory. Eq. (2.11) shows that the running coupling constant approximation can be obtained in perturbation theory if one keeps terms order $\tilde{g}^2$. The approximate running coupling $\tilde{g}_a(\lambda)$ is given in Eq. (2.12).

The question is how large are the corrections indicated in Eq. (2.13). The next Section describes our numerical study of the model.

3. NUMERICAL RESULTS

The goal of our numerical study is to understand the structure and determine the usefulness of the effective hamiltonians for the calculation of the bound state energy. We want to find out if perturbatively calculated effective hamiltonians of small width (of order 1 GeV) can reproduce the bound state eigenvalue. We are interested in perturbation theory because it is the tool we can use in the hamiltonian approach to QCD. We aim to make the width λ as small as possible because the smaller is the width the smaller basis of effective states is required to calculate the bound state eigenvalue.

The questions how small can be the width of the perturbatively calculated effective hamiltonians and how well the hamiltonians can reproduce the bound state properties, are of principal interest because the perturbative running coupling constant grows in asymptotically free theories when the width gets smaller and at some unknown point perturbation theory becomes useless.

The approximate result for the running coupling constant $\tilde{g}_a(\lambda)$ in Eq. (2.13) can be compared to the exact value of the running coupling. The exact solution is obtained by the numerical integration of the flow equation, i.e. Eq. (2.7). The numerical computations were performed using the Runge-Kutta integration algorithm of rank 4. [9] The results were obtained using two independent alghorithms. The hamiltonians were cross-checked using various theoretical conditions such as the hermiticity and width-independence of the eigenvalues.

The exact running coupling, $\tilde{g}(\lambda)$, is defined as

$$\tilde{g}(\lambda) \quad = \quad - \mathcal{H}_{M,M+1}(\lambda)/\sqrt{E_M E_{M+1}} \quad . \tag{3.1}$$

Fig. 1. shows the running coupling constants $\tilde{g}$ and $\tilde{g}_a$ as functions of the width λ. It is visible that the approximate solution blows up in the flow before the effective hamiltonian width is reduced to the scale where the bound state is formed.

The bound state formation scale is defined using the relevant effective hamiltonian matrix element $\tilde{\mu}$ which is defined as

$$\tilde{\mu}(\lambda) \quad = \quad \mathcal{H}_{-1,-1}(\lambda) \quad - \quad 0.5\,\text{GeV} \quad . \tag{3.2}$$

$\tilde{\mu}$ becomes equal -1.5 GeV when the diagonal matrix element $\mathcal{H}_{-1,-1}$ of the effective hamiltonian becomes equal to the bound state eigenvalue, -1 GeV. The width λ where the bound state eigenvalue appears on the diagonal is equal about 0.5 GeV. $\tilde{\mu}$ stays constant for smaller λ. This width scale (order 1 GeV) is called the bound state formation scale. The exact result of integrating Eq. (2.7) gives the function $\tilde{\mu}(\lambda)$ which is plotted in Fig. 1.

Fig. 1 also shows that the exact effective coupling constant is close to the one in Eq. (2.13). This is a hint for that the corrections indicated in Eq. (2.13) are small for λ larger than order 16 GeV. The effective hamiltonians for smaller λ may still have similar structure but the running coupling is not given by Eq. (2.12).

The most important feature visible in Fig. 1 is that the exact effective coupling constant does not grow unlimitedly. This encourages us to use expansion in the running coupling constant in calculations of the effective hamiltonians.

On the other hand, the diagonal matrix elements $\mathcal{D}_m = (1 - \tilde{g})E_m$ with small m become negative when $\tilde{g}$ grows above 1. [8] Thus, the absolute energy order of states is reversed. The diagonal matrix elements for states corresponding to lowest E_m become negative but

they are small in modulus. At the same time, the diagonal matrix elements for states corresponding to larger E_m become more negative. Therefore, when $\tilde{g}$ grows above 1, the states corresponding to some originally intermediate energy range become much lower on the energy scale than all other states.

This inversion feature reverses the rôle of the bilinear terms. The coupling stops growing and it begins to drop. At the same time the bound state eigenvalue is localized in the diagonal matrix element $\mathcal{H}_{-1,-1}$. This matrix element corresponds to the state which appears to be at the bottom of the energy scale. The bound state dynamics is located in matrix elements at the center of the effective hamiltonian matrix instead of the lowest indices corner, as one might expect if the lowest momentum scales were important in the bound state formation. Further renormalization group flow reduces $\tilde{g}$ below 1 and successively establishes small positive eigenvalues on the diagonal. In other words, the negative bound state eigenvalue is settled before many low positive eigenvalues are. The bound state eigenvalue appears almost independently of what happens at the bottom of the positive spectrum. This can be verified by changing M. The hamiltonian width λ limits couplings of a given state with other states to a limited number of states whose diagonal matrix elements are within the range order λ around the given state diagonal matrix element. For $b^2 = 2$ only a small number of states participate in the interaction of states with the diagonal matrix elements larger than λ. Therefore, when λ drops below the bound state formation scale, the small energy (small diagonal matrix element) states are decoupled from the bound state dynamics.

The rise of the coupling above 1 and the inversion feature suggest that even in the full hamiltonian flow the perturbative expansion is useless at the bound state formation scale. But the coupling approaches 1 from below rather smoothly. We can ask for how small λ the effective hamiltonian can be reliably calculated in perturbation theory.

Scaling symmetry in the model and Fig. 1 suggest a large range of validity of perturbation theory down to at least the width order 16 GeV where the formula (2.12) begins to fail. Namely, the hamiltonians in Eq. (2.13) possess the discrete scaling symmetry: two effective hamiltonians for two values of the width λ differing by the factor b^{-2} have matrix elements related by the shift $i \to i - 1$ and $j \to j - 1$ and replacement of $\tilde{g}(\lambda)$ by $\tilde{g}(b^{-2}\lambda)$. Thus, the flow of the effective hamiltonians is reduced to the change of the width and the coupling constant for as long as one can neglect the boundary effects due to finite N and M. Since the coupling in Eq. (2.12) is obtained keeping terms order $\tilde{g}^2$ and it runs correctly down to about 16 GeV, one can expect that Eq. (2.13) describes the effective hamiltonians correctly down to that scale.

Fig. 2 shows the bound state eigenvalue of approximate effective hamiltonians in ratio to the exact value -1 GeV, as a function of the width λ. Ratios formed this way will be used as measures of the accuracy of effective hamiltonians throught this work.

Three approximations are shown in Fig. 2. The one denoted by E results from diagonalization of hamiltonians given by Eq. (2.13) with corrections set equal 0 and inserting the exact value of $\tilde{g}(\lambda)$ for $\tilde{g}_a(\lambda)$. The curve labeled by $\mathcal{D}$ is obtained in the same way except for one modification that in the exponent E_m and E_n are multiplied by the factor $1 - \tilde{g}(\lambda)$. This multiplication replaces E_m and E_n in the exponent by $\mathcal{D}_m$ and $\mathcal{D}_n$, respectively. The intermediate curve marked g is obtained by using $\mathcal{D} = (1 - g)E$ in the exponent, i.e. the initial coupling instead of the running one.

The three curves show strong deviation from the exact eigenvalue at the beginning of the flow. This is caused by the boundary effect due to the cutoff N. The curves also deviate

from 1 at small width. This deviation shows the limited validity of the approximation. It is also clear that the gaussian similarity factor with free energies gives a better approximation than the same factor with the diagonal matrix elements.

Fig. 2 suggests that a few terms of expansion in the running coupling (e.g. only terms order 1 and $\tilde{g}$ are used in the case of curve E) may produce effective hamiltonians whose bound state eigenvalue accuracy is order 10% and whose width is smaller than 16 GeV. The amazing result is that by simply introducing the similarity function and varying the coupling one can reduce the width of the hamiltonian by a factor order 4000 and make a small error. Other eigenvalues are more accurate with the exception of eigenvalues order or larger than λ for which the approximation is not expected to work. However, the width is still quite far from the bound state formation scale. The key question now is how far down in the width one can get using an expansion in the running coupling constant.

The first comment we wish to make concerning perturbation theory is that the direct expansion in powers of the initial coupling g is not useful for calculating effective hamiltonians with small width. This is illustrated in Fig. 3 by the plot of the ratio of the effective hamiltonian bound state eigenvalue to the exact result for hamiltonians of width λ calculated using expansion into a series of powers of g up to 1, 2, 3 and 4. Note that the analogy between the model and QCD is such that g in the model corresponds to the strength of the two-particle interaction which is of the second order in QCD. Therefore, terms order g here correspond to terms order g_{QCD}^2, terms order g^2 correspond to terms order g_{QCD}^4 etc. Fig. 3 clearly demonstrates that perturbative expansions in terms of the canonical coupling constant in the initial hamiltonian are not suitable for applications in the bound state dynamics.

The reason we stress this fact here despite that such result might be expected in the lagrangian approach, is that we study a hamiltonian approach. The hamiltonian approach is different in many respects from the familiar perturbative lagrangian approaches. [1] In the light-front hamiltonian approaches, it is often silently assumed that one can analyse nonperturbative aspects of the light-front QCD hamiltonian dynamics using canonical hamiltonian terms and neglecting the running coupling effects. Fig. 3 warns us not to do so.

In contrast to Fig. 3, Fig. 4 shows results obtained from effective hamiltonians calculated in the second order expansion in terms of the effective coupling constant $\tilde{g}(\lambda_0)$, for a set of choices of λ_0. The curves are marked by the value of λ_0 in GeV. For comparison, we include the second order result of the expansion in terms of g which is marked by the sign ∞ and equals to the curve marked 2 in Fig. 3. The actual value of $\tilde{g}$ which is used to evaluate the hamiltonians $\mathcal{H}(\lambda)$ is equal to the exact value of $\tilde{g}(\lambda_0)$ in the model. In a theory where an exact solution is not known, the exact coupling constant $\tilde{g}(\lambda_0)$ is not known and its value must be fitted in $\mathcal{H}(\lambda)$ at a useful value of λ. Varying of λ should not cause significant changes if the approximation and the fit are nearly exact.

The expansion of the renormalization group flow in powers of an effective coupling $\tilde{g}(\lambda_0)$ is done in the following way. One expands the flow in powers of the initial g and computes $\tilde{g}(\lambda_0)$ as a series in g using Eq. (3.1). The latter series is inverted and g is calculated as a series in $\tilde{g}(\lambda_0)$. Then, the whole family of effective hamiltonians parametrized by λ is calculated in expansion of powers of $\tilde{g}(\lambda_0)$ by substituting the inverted series into the known expansion in powers of g.

Thus, the effective hamiltonians are calculated using expansion in powers of $\tilde{g}(\lambda_0)$. They are diagonalized and their bound state eigenvalues are plotted as functions of λ, for every single value of λ_0 we choose. It is expected that an expansion in powers of $\tilde{g}(\lambda_0)$ works only

for effective hamiltonians with widths λ in the vicinity of λ_0. This feature is clearly visible in Fig. 4 for $\lambda_0 = \infty$, 512, 32, 8, 2 and 1 GeV. The arrows in Fig. 4 show points where $\lambda = \lambda_0$.

The next question is what happens in the higher orders of perturbation theory. This question can be only partially answered on the basis of the limited numerical studies we have performed. Therefore, we limit the discussion here to the analysis of the lowest orders in the perturbative expansion for the key matrix element of Eq. (3.2) and the bound state eigenvalue.

Firstly, note that Eq. (2.12) can be viewed as a result of summing a geometric series. It is clear that when λ approaches 2 GeV, the coefficients in the expansion of $\tilde{g}_a$ in powers of g grow as powers of N. Therefore, one should expect that when $g > 1/N$ the series will not converge. The value of g we are using in the model is only a little bit smaller than $1/16$, as required by the condition for the bound state energy to be -1 GeV. For $\lambda \gg 2$ GeV the coefficients are powers of much smaller numbers than N and one can expect a small number of terms to reproduce the running coupling value, but when the width gets small, the number of terms in the expansion must become very large to reach the approximate result. When one switches to the expansion in the exact running coupling constant, the number of needed terms is unknown. We will discuss the lowest 6 terms only.

Secondly, it follows from Fig. 1 that the exact solution for $\tilde{g}(\lambda)$ is limited and always stays below 1.1, in a dramatic distinction from the approximate running coupling result which diverges below 4 GeV. This suggests that the perturbative expansion for the full hamiltonian may be extendible beyond the barrier around 4 GeV. We show below it does happen so for the first three terms in the expansion.

The difficulty we encounter with terms of higher order than $\tilde{g}^2$ can be seen still using Eq. (2.12). Suppose $\lambda = 16$ GeV. We see in Fig. 1 that the second order perturbative result for $\tilde{g}_a(16\,\text{GeV})$ is quite close to the exact coupling constant $\tilde{g}(16\,\text{GeV})$. So, let us approximate the function $\tilde{g}(\lambda)$ by the function $\tilde{g}_a(\lambda)$ for $\lambda \geq 16$ GeV. Then, using Eq. (2.12) at $\lambda = 16$ GeV, one obtains the inverse series

$$ g \;=\; \tilde{g} - (13.4\,\tilde{g})^2 + (13.4\,\tilde{g})^3 - (13.4\,\tilde{g})^4 + ... , \tag{3.3} $$

with the alternating sign. The first 6 actual coefficients which replace the successive powers of 13.4 in the full perturbative expansion are: 1.0, -13.42, 177.3, -2309, 29752 and -379277. For example, the approximation in Eq. (3.3) deviates from the actual coefficients by about 5% for the coefficient of $\tilde{g}^4$ and about 20% for $\tilde{g}^6$.

Now, let us calculate the matrix element $\tilde{\mu}(16\,\text{GeV})$ of Eq. (3.2) as a power series in g. The actual coefficients are -0.50, -6.71, -88.6, -1153, -14832 and -188759. Inserting the expansion from Eq. (3.3) one obtains the coefficients in $\tilde{\mu}(16\,\text{GeV})$ in front of the powers of $\tilde{g}(16\,\text{GeV})$, from the 1st to 6th, equal -0.5, 0.0008, 0.04, -0.14, 1.2 and -17.3, correspondingly. One can easily test the series and see that it provides a good convergent approximation to the $\tilde{\mu}(\tilde{g})$ for very small values of $\tilde{g}$, such as 0.001 or even 0.01.

The exact value of the running coupling constant, $\tilde{g}(16\,\text{GeV})$, is of the order 0.27. For this value of $\tilde{g}$ one obtains the result $\tilde{\mu}(16\,\text{GeV}) = [-0.13500 + 0.000057 + 0.00079 - 0.00074 + 0.00174 - .00671]$ GeV. This sum does not include terms order 1. The first term comes from the order $\tilde{g}$, second from $\tilde{g}^2$ etc..

It is clear now that for the first three terms order $\tilde{g}^k$ with $k = 0$, 1 and 2 we can expect convergence of the effective hamiltonian calculation while the higher orders may destroy it

if one keeps only a few terms.

The need for many orders in the expansion to reach convergence *beyond the first three terms* in the expansion can be suggested already on the basis of Fig. 1. Namely, we see that the perturbative switching of $g_a(\lambda)$ from $+\infty$ to $-\infty$ is smoothed out in the full renormalization group flow of $\tilde{g}(\lambda)$. However, the turn of the curve $\tilde{g}$ below 1 GeV is sharp and a large number of terms is required to reproduce the whole curve.

It is also visible, that the successive terms may cancel out. For example, the fourth order term may remove a large contribution of the third order term. If the numerical cancelation appears for many digits, the round off errors require a close examination.

We have not performed extended studies of the model beyond the lowest order terms. Therefore, we limit ourself to the presentation of Figs. 5 and 6 which illustrate what happens up to terms order $\tilde{g}^4$. The effective hamiltonian $\mathcal{H}(\lambda)$ is expanded in a series of powers of $\tilde{g}(\lambda)$ (i.e. the running coupling at the same value of λ).

Fig. 5 shows the accuracy of the perturbatively calculated effective hamiltonians as measured by the matrix element $\tilde{\mu}(\lambda)$ from Eq. (3.2) in ratio to the exact value. The expansion including terms order 1 and $\tilde{g}$ works with 10% or even better accuracy down to the width 1 GeV. It is also visible, that the expansion including terms order $\tilde{g}^2$ produces accuracy on the order of 3% or better down to the width order 2 GeV but the accuracy drops down significantly near 1 GeV. The third power term produces a considerable drop in the accuracy which is then partially counterbalanced by the inclusion of the fourth power term. The oscillation pattern needs further studies to explain. We have not performed such studies.

Fig. 6. shows the accuracy of the bound state eigenvalue obtained from diagonalization of the effective hamiltonians $\mathcal{H}(\lambda)$ expanded in powers of the running coupling $\tilde{g}(\lambda)$ including powers up to 1, 2, 3 and 4, respectively. The curve 1 for the first order calculation matches curve E in Fig. 2 away from the ultraviolet (left) boundary region. This feature confirms the expectation based on Figs. 1 and 2 that a low order perturbative expansion in the running coupling constant can accurately reproduce the effective hamiltonians at small width. The curve 2 represents the result of the second order expansion and shows a considerable improvement. The accuracy is about 10% or better down to the width 1 GeV which is at the edge of the bound state formation scale. The second power of $\tilde{g}$ in the model is analogous to the fourth power of the coupling constant in QCD. Thus, the analogous calculation in QCD requires the fourth order expansion of the effective hamiltonians in powers of the strong interaction coupling constant.

It is visible in Fig. 6 that for the small values of $\tilde{g}$ the perturbative expansion is convergent. However, as expected, at small widths the powers 3 and 4 of the coupling constant appear with large coefficients. The curve including terms up to the third power of $\tilde{g}(\lambda)$ falls down quite low when we substitute the exact value of the coupling.

The fourth order curve labeled 4 is ended at the bottom edge of the figure to avoid overlap with curves 1 and 2. In fact, the curve 4 continues down to about 0.53 at $\lambda = 16$ GeV, shoots back up to 0.94 at about 12 GeV, deeps down again to about 0.5 at 8 GeV and skyrockets right after 8 GeV crossing 1 and reaching about 100 at 1 GeV. This erratic behavior is clearly correlated with the pattern visible in Fig. 5.

Despite the slow convergence problem which requires further study, Figs. 1 to 6 illustrate the striking feature of the model that the bound state eigenvalue can be obtained from diagonalization of an effective hamiltonian with the width order 1 GeV with 10% accuracy.

The remaining question is how small the space of states can be on which one can project the narrow effective hamiltonian and reproduce the bound state eigenvalue by diagonalization of the projected matrix. The wave function is expected to be reproduced with a similar accuracy.

The answer is provided in Table 1. The table contains the ratio of the bound state eigenvalue obtained by the diagonalization of a small window matrix $\tilde{\mathcal{H}}(\lambda)$ whose matrix elements are the same as the matrix elements of $\mathcal{H}(\lambda)$ in the small window but they equal 0 everywhere outside the window. The indices of the window range from $\tilde{m}$ to $\tilde{n}$ including the limiting values. The bound state eigenvalue of the window is divided by the bound state eigenvalue of the whole effective hamiltonian. Table 1 gives the results obtained from $\tilde{\mathcal{H}}(1\,\mathrm{GeV})$ which is calculated in second order expansion in the running coupling constant $\tilde{g}(1\,\mathrm{GeV})$. The bound state eigenvalue of the whole effective hamiltonian $\mathcal{H}(1\,\mathrm{GeV})$ is equal $-0.8902\,\mathrm{GeV}$ (the exact value is $-1\,\mathrm{GeV}$). The entries in Table 1 show that the small window matrix easily reproduces this result with a relatively high accuracy. This is a spectacular feature of the method and the model. For the coupling constant $\tilde{g}(1\,\mathrm{GeV})$ is equal 1.05 and still the bound state eigenvalue accuracy one obtains from the small window hamiltonians calculated in second order perturbation theory is on the order of 10%.

Table 1 demonstrates that our hamiltonian approach can be used to calculate a 10×10 or even 5×5 matrix whose lowest eigenvalue reproduces the full theory bound state eigenvalue with accuracy order 10 to 20%. This model result can be viewed as encouraging to pursue a similar strategy in case of QCD. However, the slow down or absence of convergence beyond the second order expansion near the bound state formation scale, require improvements.

4. CONCLUSION

We have studied two basic approximations which may be of help in the hamiltonian calculations of bound state properties in asymptotically free theories. The first one can be briefly described as constructing effective hamiltonians by introducing the similarity factors and adjusting coupling constants. We provide the definition of the asymptotically free running coupling constant in the hamiltonian approach. The second approximation is an expansion into a series of powers of the running coupling constant. In both cases, the bound state eigenvalues and eigenstates of the full theory are found by diagonalizing the effective hamiltonians.

Our model study suggests that one may hope to calculate effective hamiltonians down to the similarity width which is close to the bound state formation scale. The coupling constant growth is limited. Moreover, the effective hamiltonian can be diagonalized in a limited subspace of states which dominate the bound state dynamics, instead of using the full basis. The small window hamiltonian reproduces the whole effective hamiltonian bound state eigenvalue with accuracy order 10% or better.

The model exhibits an inversion of the energy hierarchy of states when the coupling constant becomes slightly larger than 1. On the one hand, this feature is welcomed because it decouples the small momentum scales from the bound state dynamics. On the other hand, this feature appears at the coupling larger than 1 and it is beyond the reach of a simple perturbation theory. One can ask if a similar difficulty must exist in QCD. The expected answer is no. For one may hope that gluons effectively obtain masses already

11

at small values of the coupling constant through the gluonic couplings. These masses (or potentials) may set the states with gluons appart in energy when the width gets small before the coupling becomes too large for being treated in perturbation theory.

A comment is in order concerning the similarity approach in view of the latest findings in the lattice calculations that glueballs are unexpectedly heavy. [11] The hypothesis is that glueballs are heavy because the effective potentials binding two gluons are much stronger (perhaps by a factor of four) than the potentials that bind quarks. The reason is that gluons are in the octet representation of SU(3), which is analogous to being a doubly charged object in SU(1). Thus, if one compares a quark bound state to hydrogen, a glueball bound state is comparable to helium, but with one doubly-charged electron rather than two singly charged electrons. Obviously the helium and doubly charged electron are far more strongly bound than hydrogen is.

What this means is that as the coupling constant increases with decreasing hamiltonian width, the coupling of gluons will always be four times larger than the coupling for quarks, which suggests the gluon coupling would be expected to become strong enough to create a bound state of gluons while still too small to bind quarks. The strong gluon binding would naturally lead to a high effective mass for gluons, making them unlikely to be present in quark bound states. This would explain why we see no evidence of explicit constituent bound states involving gluons as well as quarks, yet allow the quark-quark potential to have strong higher order corrections. A major question for this picture would be to understand sum rules for deep inelastic scattering which have been interpreted as implying a large contribution from constituent gluons inside the proton. It might be that development of the similarity transformation formalism would show that sum rule data refers more to "current" quarks and gluons, before the similarity transformation is applied, rather than to constituent quarks and gluons after the transformation, where the gluon contribution could be very small by these arguments.

Our study shows that the convergence of perturbation theory is in jeopardy beyond the second order expansion for large values of the running coupling constant. Ref. [1] suggested that one can use the phenomenological success of the constituent quark model to improve convergence when solving QCD in the light-front hamiltonian approach. The improvement is expected to result from using a constituent quark hamiltonian as a first approximation to the small width effective hamiltonian of QCD. The chance exists, that such a constituent quark hamiltonian is not much different from the theoretical one in QCD. Therefore, the distance to the true effective hamiltonian may be calculable in perturbation theory. We wish to add a comment on how this suggestion could be checked numerically in the model.

The analogous step could be done in the present model in the following way. For certain λ_0 close to the bound state formation scale, order a few GeV, the running coupling, $\tilde{g}_0 \equiv \tilde{g}(\lambda_0)$, has a value comparable to 0.5. Let us denote the exact value of $\tilde{g}_0$ by g_s (s is chosen for "strong"). The perturbative expansions towards smaller widths order 1 GeV in terms of $\tilde{g}(\lambda)$ are hard to continue because of the large distance from the small coupling g in the initial hamiltonian. In these circumstances, we can add and subtract a suitable term in the hamiltonian $\mathcal{H}(\lambda_0)$, say μ_{CQM}. This step changes nothing. But we can multiply the subtracted term by the ratio $\tilde{g}_0/g_s$. For $\tilde{g}_0 = g_s$ nothing is changed in the theory. On the other hand, if we replace $\tilde{g}_0$ by a small number, the subtracted term together with the original interaction can be treated as a small perturbation. In fact, if μ_{CQM} represents the bulk of the effective hamiltonian then the difference between the effective hamiltonian and

μ_{CQM} will not lead to large corrections even if $\tilde{g}_0$ is rised to g_s. Thus, perturbation theory in terms of $\tilde{g}_0$ could be continued towards the smaller widths and the coefficients could be kept small. One can think of the hamiltonian μ_{CQM} as a matrix which has only one matrix element different from 0, right in the place on the diagonal where the bound state eigenvalue appears. Other forms are also possible. The key example is provided by the approximations shown in Fig. 2. The general feature of the example is that it amounts to the insertion of the similarity factors and adjusting the couplings.

Another opportunity for improvement in the numerical accuracy is related to the irrelevant operators. Analysis of the renormalization group equations for low energy matrix elements suggests that for small widths λ the *corrections* on the right-hand side in Eq. (2.13) should include the term $h(\lambda)$ with matrix elements of the form

$$h_{mn}(\lambda) \;=\; \frac{\tilde{h}(\lambda)}{\lambda} \, (E_m + E_n)\sqrt{E_m E_n} \; \exp\left[-[E_m - E_n]^2/\lambda^2\right] \; . \qquad (4.1)$$

A new coupling constant $\tilde{h} \sim \tilde{g}^2$ is introduced. The new term behaves as λ^{-1} for large λ and it disappears for $\lambda \to \infty$. It remains to be verified how much this term can improve the accuracy of the perturbative evaluation of narrow effective hamiltonians and the resulting bound state eigenvalues. The two couplings $\tilde{g}$ and $\tilde{h}$ are related and should be considered coherently. [12]

Too little is known yet about equations of the type (2.14) to say if they can help in accelerating convergence of the perturbative expansion.

We should mention that when b is reduced towards 1 the number of states per unit of the energy grows and the resulting matrices would have to be much larger than in the example we described. In fact, an interesting problem arises when one considers more than one state at each scale. Namely, when we have only one state per scale then no degenerate or near neighbour interactions arise. If more states appear at each scale and they couple to the near neighbours, the couplings are not reduced by the similarity transformation. The interesting question is how large can be the effective energy range of such near neighbour interactions.

References

[1] K. G. Wilson *et al.*, Phys. Rev. D**49**, 6720 (1994).

[2] St. D. Głazek and K. G. Wilson, Phys. Rev. D**48**, 5863 (1993).

[3] St. D. Głazek and K. G. Wilson, Phys. Rev. D**49**, 4214 (1994).

[4] E.g. see: D. E. Soper, Nucl. Phys. B (Proc. Suppl.) **53**, 69 (1997); M. Göckeler *et al.*, *ibid.* **53**, 81 (1997), and references therein.

[5] R. J. Perry, "A Simple Confinement Mechanism for Light-Front Quantum Chromodynamics", in "Theory of Hadrons and Light-Front QCD", Ed. St.D. Głazek, World Scientific, 1995, p. 56, and references therein; M. Brisudová and R.J. Perry, Phys. Rev. D**54**, 1831 (1996); M. Brisudová, R.J. Perry and K. G. Wilson, Phys. Rev. Lett. 78, 1227 (1997).

[6] F. Wegner, Ann. Physik **3**, 77 (1994).

[7] E.g. see R. Jackiw, in M. A. B. Bég Memorial Volume, edited by A. Ali and P. Hoodbhoy (World Scientific, Singapore, 1991), p. 25.

[8] K. G. Wilson and St. D. Głazek, to appear in "Computational Physics: Proceedings of the Ninth Physics Physics Summer School at the Australian National University", Eds. H. J. Gardner and C. M. Savage, World Scientific, Singapore 1997.

[9] W. H. Press, B. P. Flannery, S. A. Teukolsky, W.T. Vettering, "Numerical Recipes, The Art of Scientific Computing", Cambridge University Press, New York (1986), p. 355.

[10] St. D. Głazek, "Renormalization of Hamiltonians in the Light-Front Fock Space", hep-th/9706212.

[11] G. P. Lepage, private communication with one of us (KW).

[12] R. J. Perry and K. G. Wilson, Nucl. Phys. B**403**, 587 (1993).

Figure Captions

Fig. 1. The approximate running coupling $\tilde{g}_a(\lambda)$ from Eq. (2.13) and the exact running coupling $\tilde{g}(\lambda)$ from Eq. (3.1) plotted as functions of the effective hamiltonian width λ. The exact reduced matrix element $\tilde{\mu}$ from Eq. (3.2) is also plotted to show the width range where the bound state eigenvalue appears on the diagonal.

Fig. 2. The bound state eigenvalue of approximate effective hamiltonians in ratio to the exact value -1 GeV. Curve E results from Eq. (2.13) with *corrections* set equal 0. Curve $\mathcal{D}$ is obtained in the same way as E except for H_0 eigenvalues E in the Gaussian similarity factor replaced by the diagonal matrix elements of the approximate effective hamiltonian, i.e. $\mathcal{D} = (1 - \tilde{g})E$, (see the text). The intermediate curve marked g is obtained by using $\mathcal{D} = (1 - g)E$ in the exponent, i.e. the initial coupling instead of the running one.

Fig. 3. The ratio of the effective hamiltonian bound state eigenvalue to the exact result, for the hamiltonians of width λ calculated using expansion in powers of the initial coupling constant g up to 1, 2, 3 and 4, respectively. It is visible, that the expansion is not useful in the calculation of the bound state eigenvalue.

Fig. 4. The accuracy of the bound state eigenvalues obtained from effective hamiltonians whose renormalization group flow with the width λ is calculated expanding in powers of the effective coupling constant $\tilde{g}(\lambda_0)$ and including terms order 1, $\tilde{g}(\lambda_0)$ and $\tilde{g}^2(\lambda_0)$. The accuracy is given as ratio of the bound state eigenvalue obtained by diagonalization of the effective hamiltonian of width λ to the exact value, -1 GeV. The curves correspond to the indicated values of λ_0 (in units of GeV). The result of expansion in the initial coupling g is denoted by ∞. The arrows show points where $\lambda = \lambda_0$.

Fig. 5. The accuracy of the perturbatively calculated effective hamiltonians as measured by the matrix element $\tilde{\mu}(\lambda)$ from Eq. (3.2) in ratio to its exact value. The numbers label results obtained by expanding in powers of the running coupling constant $\tilde{g}(\lambda)$ including powers up to 1, 2, 3 and 4, respectively. The ratio would be indistinguishable from 1 for widths larger than 64 GeV if it were plotted in the scale of this figure.

Fig. 6. Accuracy of the bound state eigenvalue obtained from diagonalization of the effective hamiltonians $\mathcal{H}(\lambda)$ expanded in powers of the running coupling $\tilde{g}(\lambda)$ including powers up to 1, 2, 3 and 4, respectively. The curve 1 matches curve E in Fig. 2 away from the left boundary region. The curve order 2 shows 10% accuracy down to the width 1 GeV. The lack of convergence for higher order curves at small widths is discussed in the text.

Table 1. Ratio of the bound state eigenvalue of the small window hamiltonian with indices limited by $\tilde{m}$ and $\tilde{n}$, to the eigenvalue of the whole effective hamiltonian at $\lambda = 1$ GeV calculated using expansion up to second power in the running coupling $\tilde{g}(1\,\text{GeV})$. 0.993 corresponds to the absolute accuracy of the bound state eigenvalue equal 12% and 0.908 to 19% (see the text).
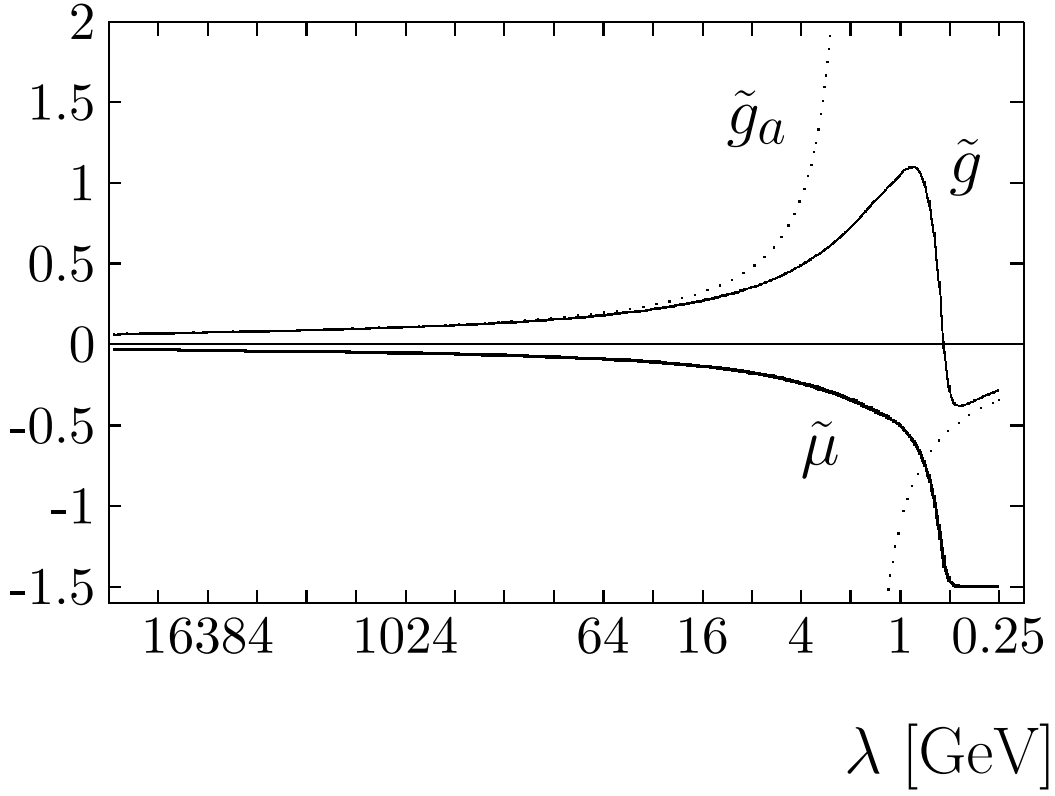
Fig. 1

Fig. 1. The approximate running coupling $\tilde{g}_a(\lambda)$ from Eq. (2.13) and the exact running coupling $\tilde{g}(\lambda)$ from Eq. (3.1) plotted as functions of the effective hamiltonian width λ. The exact reduced matrix element $\tilde{\mu}$ from Eq. (3.2) is also plotted to show the width range where the bound state eigenvalue appears on the diagonal.
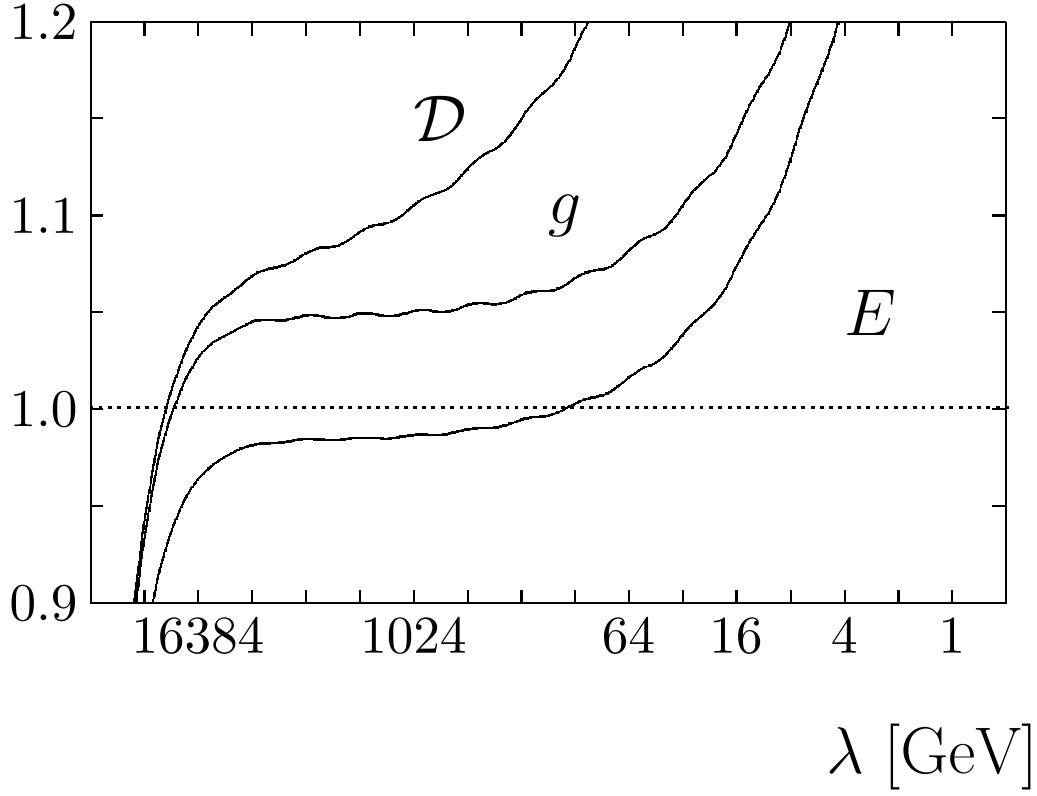
Fig. 2

Fig. 2. The bound state eigenvalue of approximate effective hamiltonians in ratio to the exact value -1 GeV. Curve E results from Eq. (2.13) with *corrections* set equal 0. Curve $\mathcal{D}$ is obtained in the same way as E except for H_0 eigenvalues E in the Gaussian similarity factor replaced by the diagonal matrix elements of the approximate effective hamiltonian, i.e. $\mathcal{D} = (1 - \tilde{g})E$, (see the text). The intermediate curve marked g is obtained by using $\mathcal{D} = (1 - g)E$ in the exponent, i.e. the initial coupling instead of the running one.
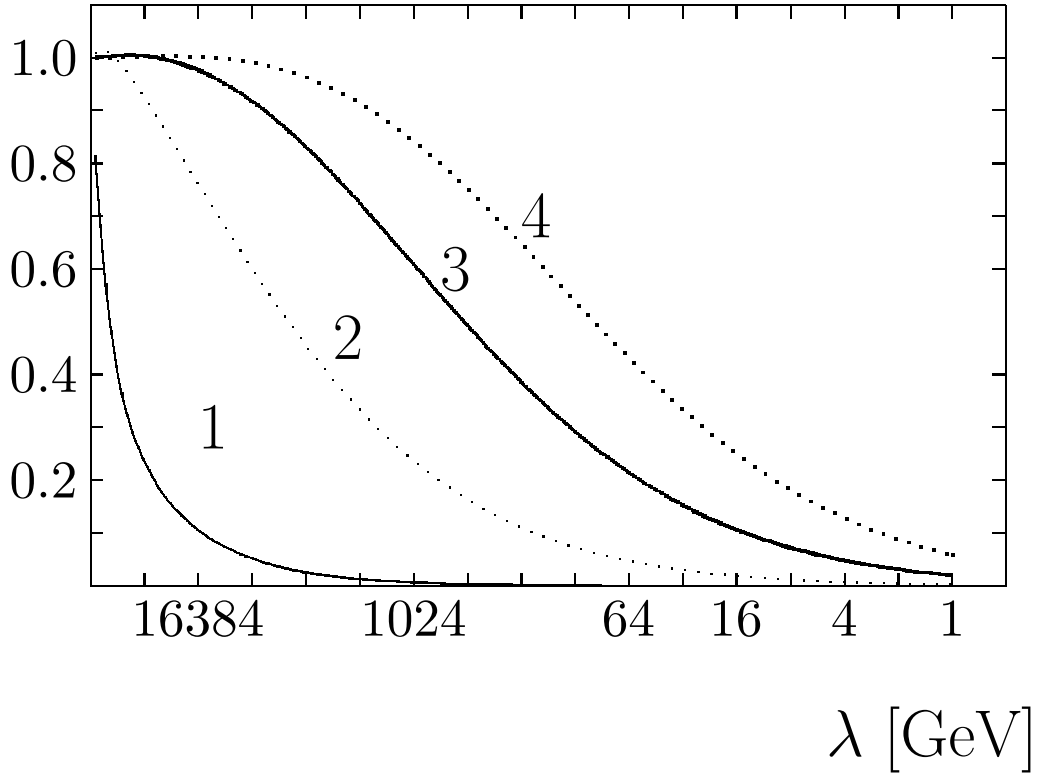
Fig. 3

Fig. 3. The ratio of the effective hamiltonian bound state eigenvalue to the exact result, for the hamiltonians of width λ calculated using expansion in powers of the initial coupling constant g up to 1, 2, 3 and 4, respectively. It is visible, that the expansion is not useful in the calculation of the bound state eigenvalue.
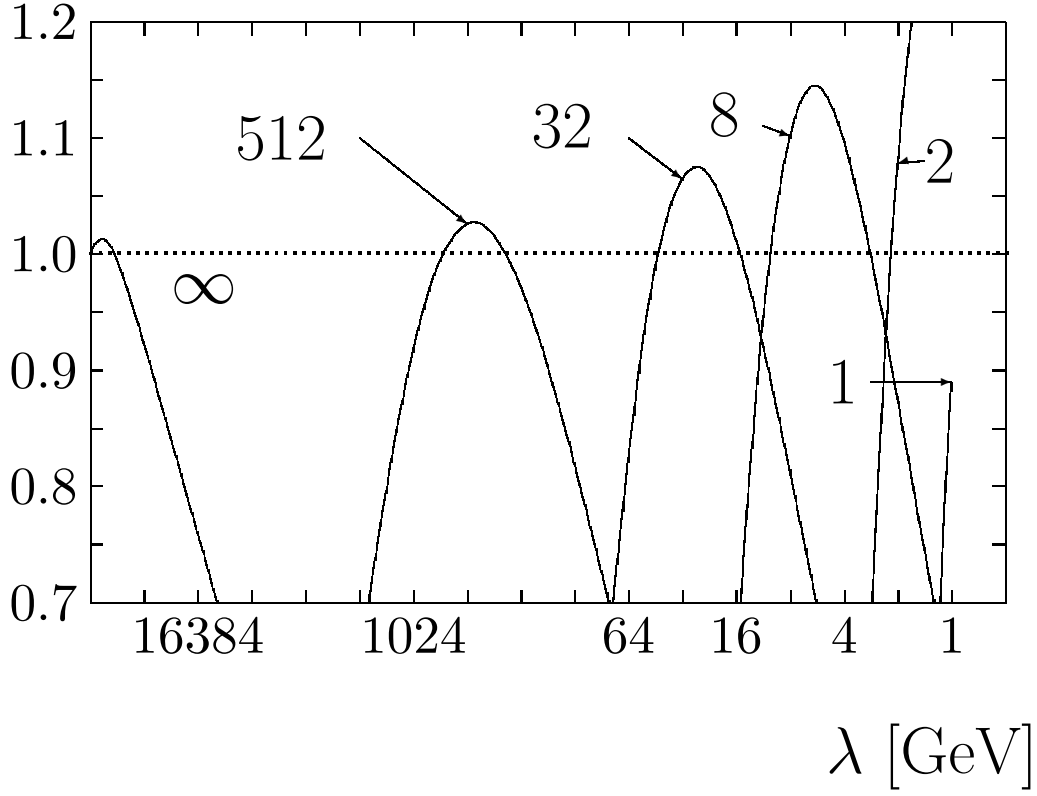
Fig. 4

Fig. 4. The accuracy of the bound state eigenvalues obtained from effective hamiltonians whose renormalization group flow with the width λ is calculated expanding in powers of the effective coupling constant $\tilde{g}(\lambda_0)$ and including terms order 1, $\tilde{g}(\lambda_0)$ and $\tilde{g}^2(\lambda_0)$. The accuracy is given as ratio of the bound state eigenvalue obtained by diagonalization of the effective hamiltonian of width λ to the exact value, -1 GeV. The curves correspond to the indicated values of λ_0 (in units of GeV). The result of expansion in the initial coupling g is denoted by ∞. The arrows show points where $\lambda = \lambda_0$.
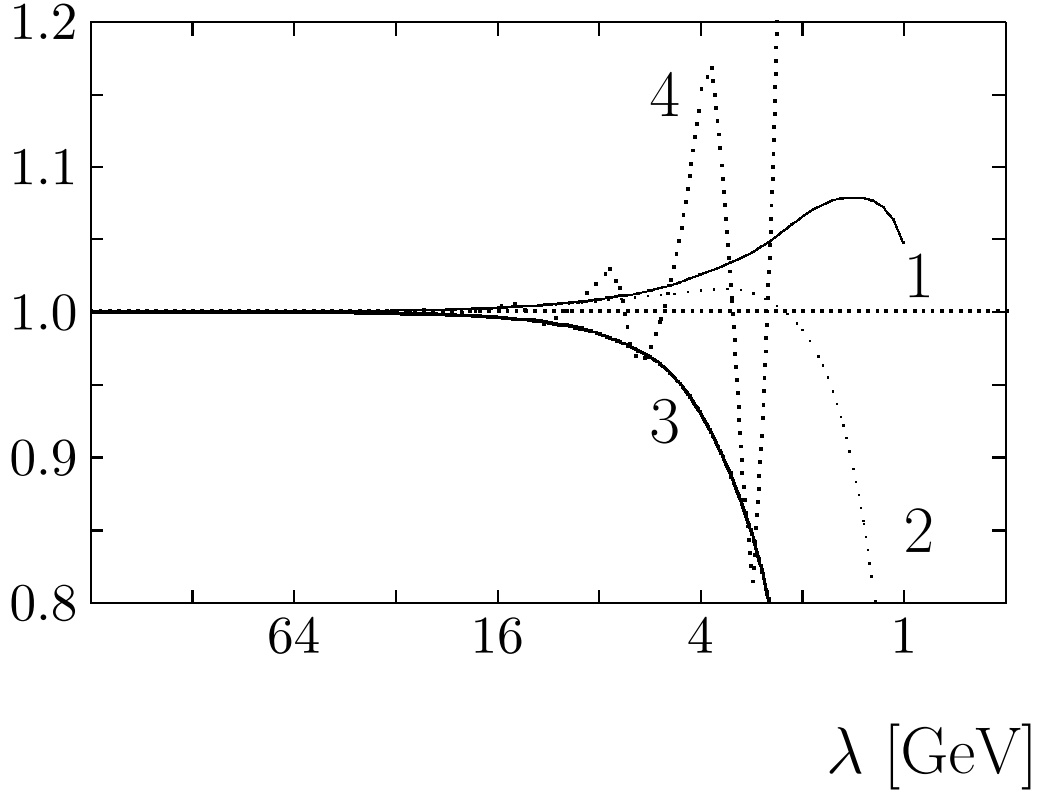
Fig. 5

Fig. 5. The accuracy of the perturbatively calculated effective hamiltonians as measured by the matrix element $\tilde{\mu}(\lambda)$ from Eq. (3.2) in ratio to its exact value. The numbers label results obtained by expanding in powers of the running coupling constant $\tilde{g}(\lambda)$ including powers up to 1, 2, 3 and 4, respectively. The ratio would be indistinguishable from 1 for widths larger than 64 GeV if it were plotted in the scale of this figure.
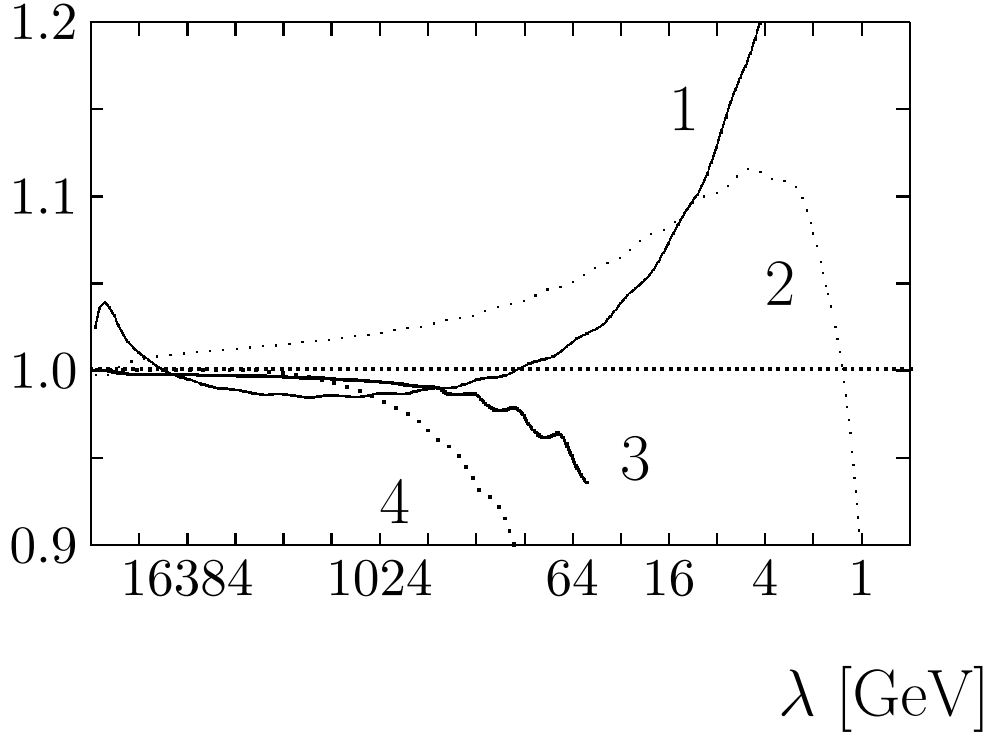
Fig. 6

Fig. 6. Accuracy of the bound state eigenvalue obtained from diagonalization of the effective hamiltonians $\mathcal{H}(\lambda)$ expanded in powers of the running coupling $\tilde{g}(\lambda)$ including powers up to 1, 2, 3 and 4, respectively. The curve 1 matches curve E in Fig. 2 away from the left boundary region. The curve order 2 shows 10% accuracy down to the width 1 GeV. The lack of convergence for higher order curves at small widths is discussed in the text.

Table 1

window/whole	$\tilde{n} = 2$	$\tilde{n} = 1$	$\tilde{n} = 0$
$\tilde{m} = -8$	0.993	0.993	0.961
$\tilde{m} = -5$	0.940	0.940	0.908

Table 1. Ratio of the bound state eigenvalue of the small window hamiltonian with indices limited by $\tilde{m}$ and $\tilde{n}$, to the eigenvalue of the whole effective hamiltonian at $\lambda = 1$ GeV calculated using expansion up to second power in the running coupling $\tilde{g}(1\text{GeV})$. 0.993 corresponds to the absolute accuracy of the bound state eigenvalue equal 12% and 0.908 to 19% (see the text).